Measurements and Models for Hazardous Chemical and Mixed Wastes

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Tank wastes contain complex mixtures with aqueous, organic and electrolyte components. In order to effectively treat, safely handle, and properly dispose of these wastes, accurate and comprehensive knowledge of the basic thermophysical properties is paramount. For instance, the vapor pressure and vapor composition over the solution is a strong function of temperature, and the vapor properties are needed to design safe tank handling procedures, and stripping operations. The complete modeling of mixed solvent (aqueous + organic) electrolyte solutions is one of the remaining fundamental problems in solution thermodynamics. In addition, measurements for these solutions are usually limited.

In this project we undertake to develop models that work well for predicting the vapor-liquid equilibria (VLE), phase density, and infinite dilution activity coefficients of mixtures of water + miscible organic solvents + salt. The model for the phase equilibria and densities of the coexisting phases uses the Peng-Robinson-Stryjek-Vera cubic equation of state for both the liquid and vapor phases. The density correction of Mathias *et al*. is applied to the liquid phase. The Wong-Sandler mixing rule is employed, with the non-random two liquid (NRTL) model used for the activity coefficient contribution to the mixing rules. This allows the cubic equation of state to be used for mixtures containing salts and potentially other non-volatile components.

The models developed are tested with the system water + acetone+ isopropyl alcohol + sodium nitrate. This system was selected to contain industrially important solvents with a variety of functional groups. Both literature data and newly measured properties are used for the model evaluation and development. A comparison of our modeling results to the data available in the literature and our data is also given.